

STATISTICAL METHODOLOGY
FOR DETERMINING CONTAMINANTS OF CONCERN
BY COMPARISON OF BACKGROUND AND SITE DATA
WITH APPLICATIONS TO OPERABLE UNIT 2

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Executive Summary

Statistical methodology for comparing background and site data is proposed. If levels of an analyte are statistically significantly greater in the site data the analyte is classified as a contaminant of concern (COC). The methodology is applied to seep and stream locations in Operable Unit 2 (OU2). Lists of resulting COC's for volatile organic analytes (VOA's) and semi-volatile organic analytes (SVOA's), radionuclides (RADS), total metals, dissolved metals, and water quality parameters are given in tables beginning on page 9. Problems with using tolerance intervals in such applications are also discussed.

Introduction

The statistical determination of contaminants of concern through comparisons of background and site data can be complicated by the presence of nondetects at multiple detection limits. The discussion of a generally applicable approach which is appropriate for use under these conditions begins on page 24. Copies of a branching flow chart for selecting appropriate methodology are included with discussion beginning on page 3. COC results for VOA's and SVOA's, RADS, total metals, dissolved metals, and water quality parameters are presented in tables beginning with their explanation on page 7.

While the use of tolerance limits to compare background and site locations in the determination of COC's has been given considerable attention by personnel at Rocky Flats, this approach is not appropriate for this application. It may be appropriate for the continued monitoring of sites for compliance. A discussion supporting this position is provided on pages 27 through 29.

General Discussion

The statistical methodology proposed in this report and applied to seep and stream locations in OU2 assumes that a single set of background data is being compared to a single set of site data to determine if the level of a specific analyte is elevated in the site data relative to the background data. If such an elevated level is found to be statistically significant, the analyte is designated as a contaminant of concern (COC) for the site.

If multiple sampling locations are available for potential background data, preliminary investigations should check for differences between the locations before grouping them. If such differences are found, discussion as to what constitutes the true background is required. If multiple sampling locations are available for the site data, consideration should be given to grouping or stratifying these locations into separate sites and comparing each resulting site to its appropriate background. Single locations could serve as individual sites, and that is the approach used in this report.

Three sampling locations within OU2 are investigated using the proposed methodology. Surface Water Division (SWD) personnel recommended that the three locations be considered separately. Location SW059 is classified as a seep, and seep background data is available from the three locations SW080, SW104, and SW108. SW108 is on the north side of the Rocky Flats plant while the other two locations are on the south side of the plant. Since considerable differences

within these three potential background locations are apparent only the north location SW108 is used as background for the OU2 seep location. This approach was supported in discussions with SWD personnel. Unfortunately this results in minimal amounts of background data for some of the analytes considered.

Locations SW061 and SW132 are classified as stream locations and they are compared individually to the combined four background stream locations SW004, SW005, SW006 and SW007 (from Rock Creek). Generally no differences within these four background locations were apparent so their data are grouped into a single set of background data.

Note also the discussion of Type I and Type II errors on page 27. For the following discussion on proposed methodology it is sufficient that the reader understand that small p-values (from 0.0 up to and including 0.05) indicate the associated analyte should be considered a COC while larger p-values (from more than 0.05 to 1.0) indicate the analyte is not a COC.

Discussion of Environmental COC Determination Statistical Analysis Flow Chart

Two copies of a proposed flow chart for selecting appropriate statistical methodology for COC determination are provided in this report. The first is on the following page and contains labels (circled letters) for the purposes of explaining the various steps of the flow chart. It also contains labels (circled numbers) which will be used to indicate which branch applied for a specific analyte and resulted in a COC or non-COC decision. A second copy of the flow chart without the labels follows the first.

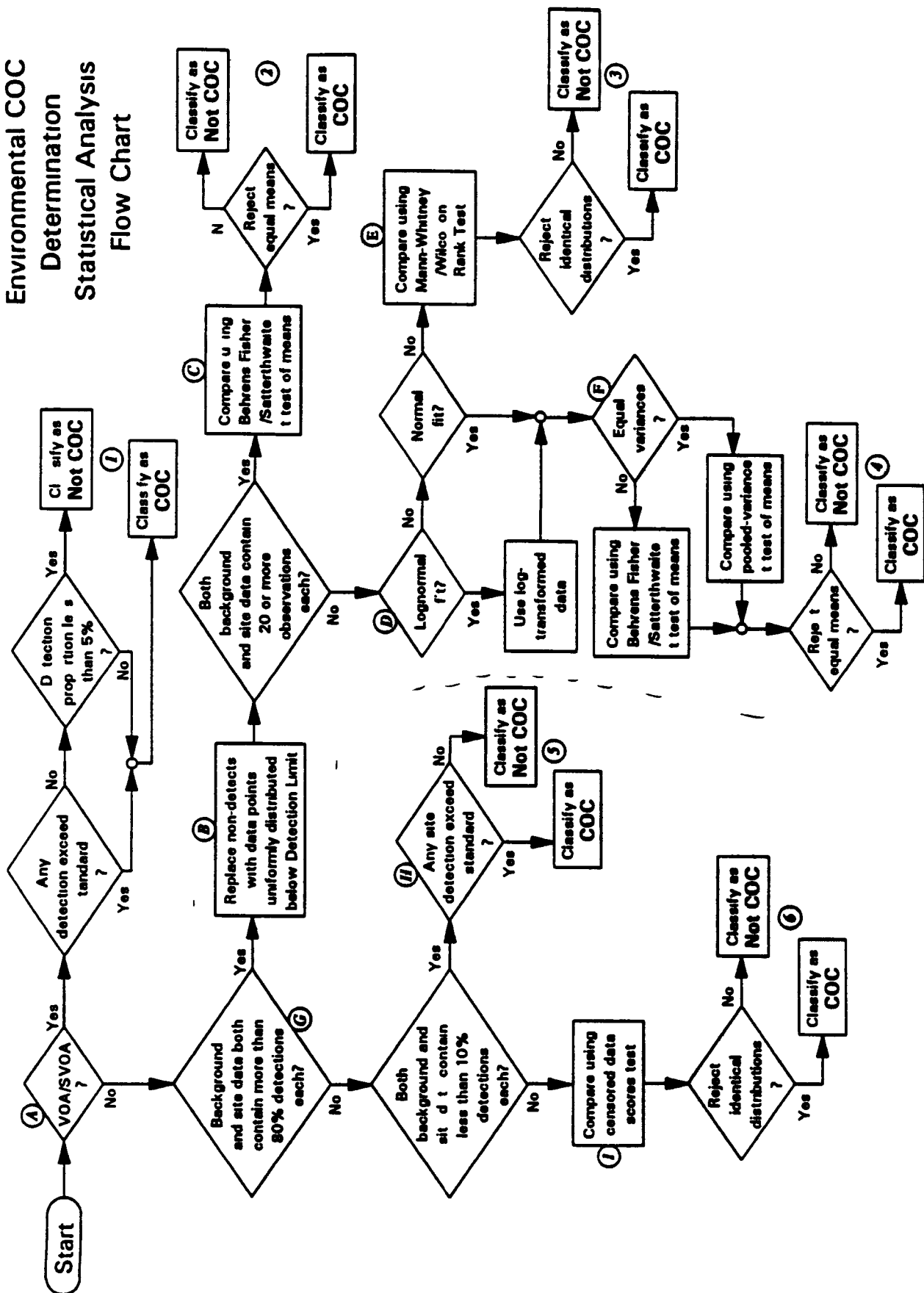
Explanations of steps labeled with circled letters A through I on the labeled flow chart are given in the following discussion.

A) Background data are not used for statistical VOA/SVOA comparisons since these analytes should not be present in background areas in any amounts. Only rarely is a detect found in the background locations used for this report. The COC criteria of five percent or more detects or any exceedance of a standard have been recommended by SWD personnel. Nondetects consist of either a U lab qualifier (analyzed for but not detected) or a J lab qualifier (estimated result less than contracted detection limit).

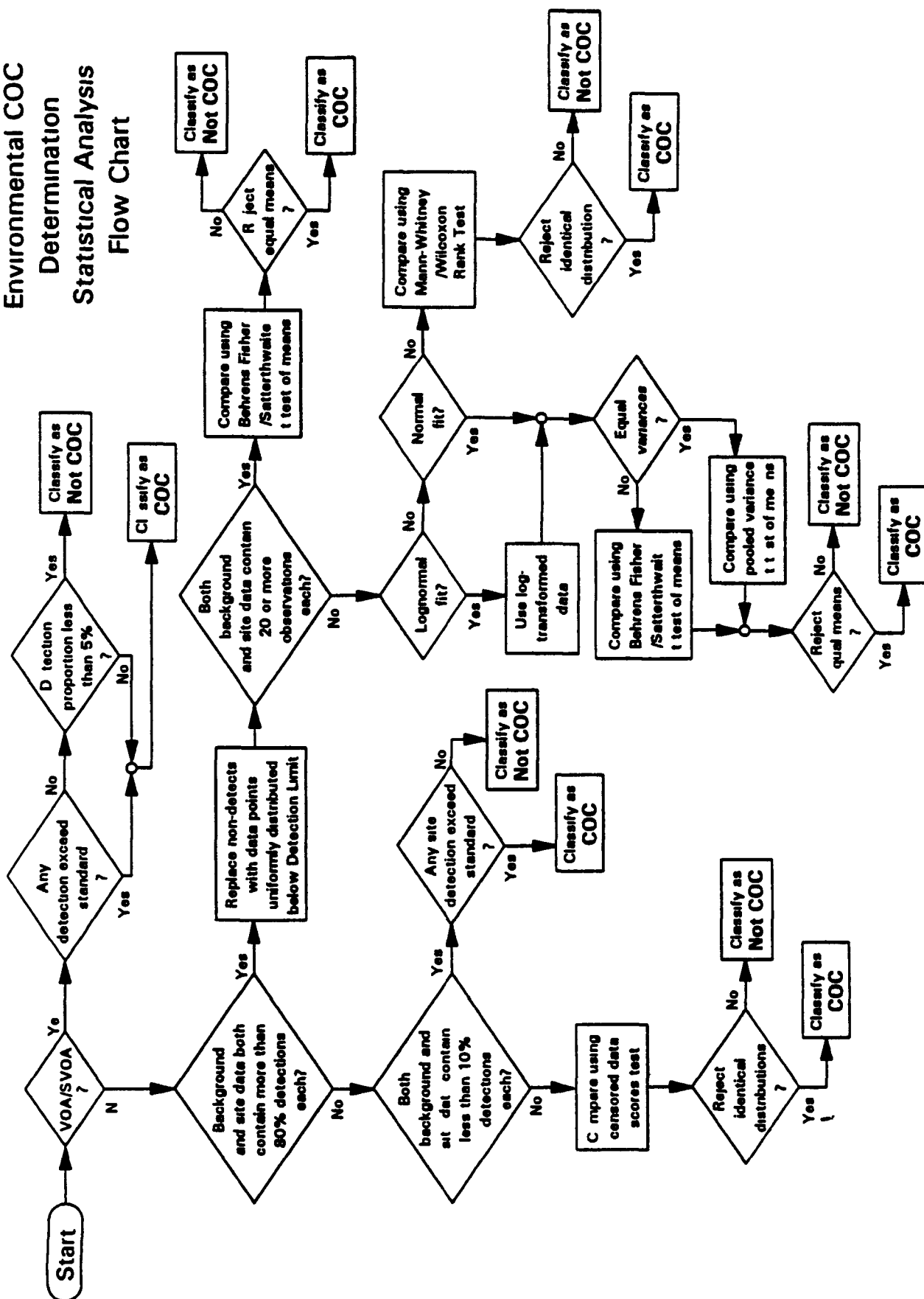
B) When both background and site data sets contain 20 percent or fewer nondetects the methodology used for COC determination is expected to be relatively insensitive to the treatment of the nondetects. The 20 percent level is fairly arbitrary; that is, no statistical criteria exist that say 20 percent is acceptable while 21 percent is not. The EPA guidelines typically recommend 15 percent as the cutoff and this level could be used instead but it is similarly arbitrary. Nondetects in this context are taken to mean censored measurements with lab qualifier U.

Since the treatment of nondetects in this case will have little impact on COC determination, simple uniform replacement of the nondetects is used primarily to facilitate goodness-of-fit results. If for example three nondetects for data from a location are at the same detection limit, say at 10.0, the three

Environmental COC Determination Statistical Analysis Flow Chart



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replacement values will be taken to be 2.5, 5.0 and 7.5. Nondetects at other levels are replaced similarly. Single nondetects are thus replaced at the detection limit divided by 2. With this approach, stacks of nondetects at the same limit will not be replaced by a common value which could result in otherwise unjustified rejection of normality or lognormality in subsequent goodness-of-fit tests.

C) When both background and site data sets contain 20 or more observations, the Central Limit Theorem can be taken to apply for the comparison of means. Use of the Behrens-Fisher t-statistic is the standard approach applied. It uses separate estimates of the two variances, so equality of the variances is not an issue. The standard Satterthwaite approximation to the degrees of freedom of this statistic using unequal variances will be sufficiently large due to the large sample sizes that normal probabilities are essentially being used.

D) Since the distributions of environmental data are often lognormally shaped, initially a log transform is made, and the residuals obtained by subtracting the respective estimated means are combined in a test for normality. Since sample sizes are small, little power in rejecting normality would be obtained if the samples were tested individually. For this reason, the testing is done on the combined residuals. If lognormality is rejected, the original untransformed data are similarly tested for normality.

E) If neither normality nor lognormality are found to be appropriate, the nonparametric Mann-Whitney/Wilcoxon rank test is used. The issue of multiple detection limits prohibiting accurate ranking of values is avoided through the uniform replacement approach discussed in note B. Again, with relatively few nondetects, the impact of such replacement on the rank test results should be minimal.

F) When either normality or lognormality appears reasonable, the standard F-test for equal variances from two normal populations is used to determine the appropriate t-statistic computational method. For unequal variances, as in part C above, the standard Behrens-Fisher t-statistic (separate variance estimates) and the Satterthwaite approximation to the degrees of freedom of the t-statistic are used. For equal variances, the standard pooled variance estimate t-statistic is used.

G) If more than 20 percent of either the background or site data sets consist of nondetects, the practice of replacing them to facilitate the determination of COCs becomes questionable (again, the actual 20 percent level is somewhat arbitrary, but a line needs to be drawn somewhere).

H) If neither the background nor site data sets contain at least 10 percent detects, insufficient information is available to support a meaningful statistical determination. For this reason, a simple convention is taken: if the site data contains any exceedances of an analyte's standard, the analyte is designated a potential COC.

I) This situation of having between 20 and 90 percent nondetects is complicated by the fact that invariably multiple detection limits are involved. If only a single detection limit were present, fairly routine parametric or nonparametric statistical methods that deal with censored data could be applied. The only technically defensible approach found by Statistical Applications personnel involves the use of a nonparametric censored data scores approach that makes use of the information available in the presence of multiple detection limits. This approach is discussed more thoroughly beginning on page 24 of this report.

Observation The branch of the flow chart starting with the B heading contains several drawbacks. Nondetect replacement, goodness-of-fit testing after replacement, outlier influence, and log transformations with possible negative data values are all aspects that diminish the statistical rigor of this section of the flow chart. Note that the scores approach (heading I) is appropriate for all cases in this branch and in fact, with no nondetects, it reduces to the Mann-Whitney/Wilcoxon approach used in the nonparametric portion of the branch.

While application of the scores approach always entails the same single step, the B-heading branch can require any or all of: data replacement, sample size consideration, log transformation, lognormal goodness-of-fit, normal goodness-of-fit, variance test, and the appropriate parametric or nonparametric test. In addition, outlier treatment can have considerably more impact on t-test results in this branch than for nonparametric methods.

Consideration should thus be given to simply always using the scores approach to avoid the difficulties commonly present in environmental data as well as the extensive sequence of analysis steps required. The scores approach will likely lead to the same COC discussion as the branching methodology, and it is more defensible as being technically correct. A discussion of how the COC determination results in this report would change if the scores approach had been used instead of the flow chart branching approach begins on page 26.

COC Results Tables

Summaries of COC results are presented in the following tables. The COC Decision Class given in the tables refers to the circled numbers from the flow chart on page 4 associated with the individual COC criterion which is applicable to the analyte for the site comparison considered. The classes are as follows:

- | | | |
|-----|---|---|
| 1 | - | VOA/SVOA detect/exceedance criteria |
| 2 | - | Large sample central limit theorem t-test |
| 3 | - | Mann-Whitney/Wilcoxon nonparametric test |
| 4Le | - | Small sample equal variance t-test under lognormality |
| 4Lu | - | Small sample unequal variance t-test under lognormality |
| 4Ne | - | Small sample equal variance t-test under normality |
| 4Nu | - | Small Sample unequal variance t-test under normality |
| 5 | - | Fewer than 10 percent detect criteria |
| 6 | - | Nonparametric censored data scores test |

Recall that when statistical tests generate p-values of 0.05 or less the associated analyte is taken to be a COC. Thus in the tables listing COC's p-values will be accordingly small they will be large in the tables listing other analytes.

Note that as with any statistical activity the impact of outlying values on conclusions should be considered. For COC determination applications outlying background values with a resulting COC determination or outlying site values with a resulting non-COC determination are not of concern since in these cases deletion of the outlier(s) would likely not change the COC determination. However with outlying background values and a resulting non-COC determination or with outlying site values and a resulting COC determination the determination may be a direct result of the outlying values. In such cases the validity of the outlying values deserves special scrutiny. If either of these situations arose during the COC determination activity in this report the cases are so indicated with an asterisk by the associated p-value column entry.

The following provides a list of table topics and where the tables are located.

Tables 1A and 1B - VOA and SVOA COC's and Others - pages 9, 10, and 11. COC's are given in Table 1A since comparisons to background data were not made. COC analytes have either more than 5 percent detects or an exceedance of the standard per COC Decision Class 1. All analytes are listed in Table 1B.

Tables 2A and 2B - Total RADS COC's and Others - pages 12 and 13. Note that the radionuclide analytes Plutonium-238, Radium-226, and Radium-228 are not included due to insufficient data.

Tables 3A, 3B, and 3C - Total Metals COC's, potential COC's, and other - pages 14 through 18. Table 3B contains potential COC's per COC Decision Class 5 that is with too few detects for a statistical comparison; an analyte with any exceedances of its standard are listed.

Tables 4A and 4B - Dissolved Metals COC's and others - pages 19 through 22. None of the dissolved metal analytes were determined to be potential COC's through COC Decision Class 5.

Table 5 - Water Quality Parameters - page 23. The only water quality parameters for which site data are available are Chloride and Total Organic Carbon.

Table 1A

OU2 VOLATILE & SEMI-VOLATILE ORGANIC COMPOUNDS

CONTAMINANTS OF CONCERN

Site	Analyte	Standard ($\mu\text{g/l}$)	Sample Size	Number of Detects	Percent Detects	Number of Exceedances
SW059	1 1 1 TRICHLOROETHANE	200 0	49	43	86 2	0
	1 1 DICHLOROETHANE		47	9	19 1	0
	1 1 DICHLOROETHENE	0 057	49	20	40 8	20
	1 2 DICHLOROETHANE	0 4	48	1	2 1	1
	1 2 DICHLOROETHENE		47	36	76 6	0
	ACETONE		46	6	13 0	0
	CARBON TETRACHLORIDE	18 0	49	48	98 0	47
	CHLOROFORM	6 0	49	48	98 8	46
	METHYLENE CHLORIDE	4 7	47	7	14 9	7
	TETRACHLOROETHENE	0 8	49	47	95 9	47
	TRICHLOROETHENE	66 0	49	47	95 9	26
	VINYL CHLORIDE	2 0	47	3	6 4	3
SW061	1 1 1 TRICHLOROETHANE	200 0	50	7	14 0	0
	1 1 DICHLOROETHENE	0 057	49	2	4 1	2
	1 2 DICHLOROETHENE		49	33	67 3	0
	ACETONE		48	5	10 4	0
	CARBON TETRACHLORIDE	18 0	50	27	54 0	2
	CHLOROFORM	6 0	50	2	4 0	1
	METHYLENE CHLORIDE	4 7	49	5	10 2	5
	TETRACHLOROETHENE	0 8	50	18	36 0	18
	TRICHLOROETHENE	66 0	50	23	46 0	1
	VINYL CHLORIDE	2 0	49	2	4 1	2
SW132	1 2 DICHLOROETHENE		28	13	46 4	0
	ACETONE		25	5	20 0	0
	METHYLENE CHLORIDE	4 7	28	5	17 9	5

Table 1B
(First of two pages)

OU2 VOLATILE & SEMI-VOLATILE ORGANIC COMPOUNDS

Analyte	Standard (µg/l)	Site SW059			Site SW061			Site SW132		
		Sample Size	Detects Qty	Pct	Sample Size	Detects Qty	Pct	Sample Size	Detects Qty	Pct
1 1 2 2 TETRACHLOROETHANE	76 00	47	0	0 0	49	0	0 0	28	0	0 0
1 1 1 TRICHLOROETHANE	200 00	49	COC		50	COC		28	0	0 0
1 1 2 TRICHLOROETHANE	0 60	48	0	0 0	50	0	0 0	28	0	0 0
1 2 4 TRICHLOROBENZENE		6	0	0 0	6	0	0 0	1	0	0 0
1 1 DICHLOROETHANE		47	COC		49	1	2 0	28	0	0 0
1 1 DICHLOROETHENE	0 057	49	COC		49	COC		27	0	0 0
1 2 DICHLOROETHENE		47	COC		49	COC		28	COC	
1 2 DICHLOROBENZENE	620 00	6	0	0 0	6	0	0 0	1	0	0 0
1 2 DICHLOROETHANE	0 40	48	COC		50	0	0 0	28	0	0 0
1 2 DICHLOROPROPANE	0 56	47	0	0 0	49	0	0 0	28	0	0 0
1 2 DIMETHYLBENZENE		0	0		3	0	0 0	0	0	
1 3 DICHLOROBENZENE	400 00	6	0	0 0	6	0	0 0	1	0	0 0
1 4 D'CHLOROBENZENE	75 00	6	0	0 0	6	0	0 0	1	0	0 0
2 4 5 TRICHLOROPHENOL		6	0	0 0	6	0	0 0	1	0	0 0
2 4 6 TRICHLOROPHENOL	2 00	6	0	0 0	6	0	0 0	1	0	0 0
2 4 DICHLOROPHENOL	21 00	6	0	0 0	6	0	0 0	1	0	0 0
2 4 DIMETHYLPHENOL	2120 00	6	0	0 0	6	0	0 0	1	0	0 0
2 4 DINITROPHENOL	14 00	5	0	0 0	4	0	0 0	1	0	0 0
2 4 DINITROTOLUENE	0 11	6	0	0 0	5	0	0 0	1	0	0 0
2 6 DINITROTOLUENE	230 00	6	0	0 0	6	0	0 0	1	0	0 0
2 BUTANONE		45	0	0 0	48	1	2 1	28	1	3 6
2 CHLOROETHYL VINYL ETHER		1	0	0 0	4	0	0 0	0	0	
2 CHLORONAPHTHALENE		6	0	0 0	6	0	0 0	1	0	0 0
2 CHLOROPHENOL	1 00	6	0	0 0	6	0	0 0	1	0	0 0
2 HEXANONE		46	0	0 0	49	1	2 0	28	0	0 0
2 METHYLNAPHTHALENE		6	0	0 0	6	0	0 0	1	0	0 0
2 METHYLPHENOL		6	0	0 0	6	0	0 0	1	0	0 0
2 NITROANILINE		6	0	0 0	6	0	0 0	1	0	0 0
2 NITROPHENOL		6	0	0 0	6	0	0 0	1	0	0 0
3 3 DICHLOROBENZIDINE		6	0	0 0	6	0	0 0	1	0	0 0
3 NITROANILINE		6	0	0 0	5	0	0 0	1	0	0 0
4 6 DINITRO 2 METHYLPHENOL		6	0	0 0	4	0	0 0	1	0	0 0
4 BROMOPHENYL PHENYL ETHER		6	0	0 0	6	0	0 0	1	0	0 0
4 CHLORO 3 METHYLPHENOL	30 00	6	0	0 0	6	0	0 0	1	0	0 0
4 CHLOROANILINE		6	0	0 0	5	0	0 0	1	0	0 0
4 CHLOROPHENYL PHENYL ETHER		6	0	0 0	6	0	0 0	1	0	0 0
4 METHYL 2 PENTANONE		46	0	0 0	49	1	2 0	28	0	0 0
4 METHYLPHENOL		6	0	0 0	6	0	0 0	1	0	0 0
4 NITROANILINE		6	0	0 0	4	0	0 0	1	0	0 0
4 NITROPHENOL		6	0	0 0	5	0	0 0	1	0	0 0
ACENAPHTHENE	520 00	6	0	0 0	6	0	0 0	1	0	0 0
ACENAPHTHYLENE	0 0028	6	0	0 0	6	0	0 0	1	0	0 0
ANTHRACENE	0 0028	6	0	0 0	6	0	0 0	1	0	0 0
A'ETONE		46	COC		48	COC		25	COC	
BFNZENE	1 00	47	0	0 0	49	0	0 0	28	0	0 0
BFNZO(a)ANTHRACENE	0 0028	6	0	0 0	6	0	0 0	1	0	0 0
BENZO(a)PYRENE	0 0028	6	0	0 0	6	0	0 0	1	0	0 0
BENZO(b)FLUORANTHENE	0 0028	6	0	0 0	6	0	0 0	1	0	0 0
BENZO(gh)PERYLENE	0 0028	6	0	0 0	6	0	0 0	1	0	0 0
BENZO(k)FLUORANTHENE	0 0028	6	0	0 0	6	0	0 0	1	0	0 0
BENZOIC ACID		5	0	0 0	4	0	0 0	1	0	0 0
BENZYL ALCOHOL		6	0	0 0	5	0	0 0	1	0	0 0

COC Indicates Contaminant of Concern (Refer to Table 1A for Analytic Results)

Table 1B
(Second of two pages)

OU2 VOLATILE & SEMI-VOLATILE ORGANIC COMPOUNDS

Analyte	Standard (µg/l)	Site SW059			Site SW061			Site SW132		
		Sample Size	Detects Qty	Pct	Sample Size	Detects Qty	Pct	Sample Size	Detects Qty	Pct
BIS(2 CHLOROETHOXY)METHANE		6	0	0 0	6	0	0 0	1	0	0 0
BIS(2 CHLOROETHYL)ETHER	0 03	6	0	0 0	6	0	0 0	1	0	0 0
BIS(2 CHLOROISOPROPYL)ETHER	1400 00	6	0	0 0	6	0	0 0	1	0	0 0
BIS(2 ETHYLHEXYL)PHTHALATE	1 80	6	0	0 0	6	0	0 0	1	0	0 0
BROMODICHLOROMETHANE	0 30	47	0	0 0	49	0	0 0	28	0	0 0
BROMOFORM	4 00	47	0	0 0	49	0	0 0	28	0	0 0
BROMOMETHANE		46	0	0 0	49	0	0 0	28	0	0 0
BUTYL BENZYL PHTHALATE	3000 00	6	0	0 0	6	0	0 0	1	0	0 0
CARBON DISULFIDE		48	0	0 0	48	0	0 0	28	0	0 0
CARBON TETRACHLORIDE	18 00	49	COC		50	COC		28	0	0 0
CHLOROBENZENE	100 00	47	0	0 0	49	1	2 0	28	0	0 0
CHLOROETHANE		46	0	0 0	48	0	0 0	28	0	0 0
CHLOROFORM	6 00	49	COC		50	COC		28	0	0 0
CHLOROMETHANE		47	0	0 0	48	0	0 0	27	0	0 0
CHRYSENE	0 0028	6	0	0 0	6	0	0 0	1	0	0 0
DI n BUTYL PHTHALATE	2700 00	6	0	0 0	6	0	0 0	1	0	0 0
D' n OCTYL PHTHALATE		6	0	0 0	6	0	0 0	1	0	0 0
DIBENZO(a h)ANTHRACENE	0 0028	6	0	0 0	6	0	0 0	1	0	0 0
DIBENZOFURAN		6	0	0 0	6	0	0 0	1	0	0 0
DIBROMOCHLOROMETHANE	6 00	47	0	0 0	49	0	0 0	28	0	0 0
DIETHYL PHTHALATE	23000 00	6	0	0 0	6	0	0 0	1	0	0 0
DIMETHYL PHTHALATE	313000 00	6	0	0 0	6	0	0 0	1	0	0 0
ETHYLBENZENE	680 00	48	0	0 0	49	0	0 0	28	0	0 0
FLUORANTHENE	42 00	6	0	0 0	6	0	0 0	1	0	0 0
FLUORENE	0 0028	6	0	0 0	6	0	0 0	1	0	0 0
HEXACHLOROBENZENE	0 00072	6	0	0 0	6	0	0 0	1	0	0 0
HEXACHLOROBUTADIENE	0 45	6	0	0 0	6	0	0 0	1	0	0 0
HEXACHLOROCYCLOPENTADIENE	5 00	6	0	0 0	6	0	0 0	1	0	0 0
HEXACHLOROETHANE	1 90	6	0	0 0	6	0	0 0	1	0	0 0
INDENO(1 2 3 cd)PYRENE	0 0028	6	0	0 0	6	0	0 0	1	0	0 0
ISOPHORONE	8 40	6	0	0 0	6	0	0 0	1	0	0 0
METHYLENE CHLORIDE	4 7	47	COC		49	COC		28	COC	
N NITROSO DI n PROPYLAMINE	0 01	6	0	0 0	6	0	0 0	1	0	0 0
N NITROSODIPHENYLAMINE	4 90	6	0	0 0	6	0	0 0	1	0	0 0
NAPHTHALENE	0 0028	6	0	0 0	6	0	0 0	1	0	0 0
NITROBENZENE	3 50	6	0	0 0	6	0	0 0	1	0	0 0
PENTACHLOROPHENOL	5 70	6	0	0 0	6	0	0 0	1	0	0 0
PHENANTHRENE	0 0028	6	0	0 0	6	0	0 0	1	0	0 0
PHENOL	2560 00	6	0	0 0	6	0	0 0	1	0	0 0
PYRENE	0 0028	6	0	0 0	6	0	0 0	1	0	0 0
STYRENE		47	0	0 0	49	0	0 0	28	0	0 0
TETRACHLOROETHENE	0 80	49	COC		50	COC		28	0	0 0
TIC		1	0	0 0	3	0	0 0	1	0	0 0
TOLUENE	1000 00	47	0	0 0	49	2	4 1	28	0	0 0
TOTAL XYLENES		47	0	0 0	49	0	0 0	28	0	0 0
TRICHLOROETHENE	66 00	49	COC		50	COC		28	0	0 0
VINYL ACETATE		44	0	0 0	49	0	0 0	28	0	0 0
VINYL CHLORIDE	2 00	47	COC		49	COC		28	0	0 0
cis 1 3 DICHLOROPROPENE	10 00	48	0	0 0	49	0	0 0	28	0	0 0
trans 1 2 DICHLOROETHENE	100 00	1	0	0 0	1	0	0 0	0	0	
trans 1 3 DICHLOROPROPENE		47	0	0 0	49	0	0 0	28	0	0 0

COC Indicates Contaminant of Concern (Refer to Table 1A for Analytic Results)

Table 2A

OU2 TOTAL RADIONUCLIDES - CONTAMINANTS OF CONCERN

Site	Analyte	Background Sample Size	Site Sample Size	COC Decision Class	p Value
SW059	Americium 241	9	19	3	0 0079
	Plutonium 239,240	9	22	4Le	0 0001
	Uranium Total	2	23	3	0 0443
	Uranium 233,234	7	15	3	0 0062
	Uranium 235	6	15	3	0 0397
	Uranium 238	7	15	3	0 0062
SW061	Americium 241	45	27	2	0 0439
	Plutonium 239,240	45	27	2	0 0006
	Tritium	27	11	3	0 0044
	Uranium Total	10	28	3	0 0009
	Uranium 233 234	33	20	2	0 0001
	Uranium 235	30	20	2	0 0008
	Uranium 238	30	20	2	0 0001
SW132	Americium 241	45	19	3	0 0002
	Plutonium 239 240	45	19	3	0 0011
	U a um, Total	10	22	4Nu	0 0001
	Uranium 233,234	33	14	4Le	0 0000
	Uranium 235	30	14	3	0 0047
	Uranium 238	30	14	4Le	0 0000

Analyte would not be declared a COC if site observation SW05990001 were deleted

Table 2B

OU2 TOTAL RADIONUCLIDES - OTHERS

Site	Analyte	Background Sample Size	Site Sample Size	COC Decision Class	p Value
SW059	Cesium 137	11	18	4Ne	0.5799
	Strontium 89 90	9	17	4Lu	0.3106
	Tritium	8	12	4Le	0.3811
SW061	Cesium 137	40	19	3	0.5804
	Strontium 89 90	35	20	2	0.9832
SW132	Cesium 137	40	11	3	0.4276
	Strontium 89 90	35	11	4Le	0.8306
	Tritium	27	4	3	0.1133

Table 3A

OU2 TOTAL METALS - CONTAMINANTS OF CONCERN

Site	Analyte	Background		Site		COC Decision Class	p Value
		Sample Size	% Detects	Sample Size	% Detects		
SW059	Barium	14	85.7	37	94.6	3	0.0002
	Calcium	17	100.0	37	100.0	3	0.0005
	Magnesium	18	100.0	37	100.0	4Ne	0.0001
	Sodium	18	100.0	37	100.0	3	0.0001
	Strontium	15	80.0	37	100.0	4Lu	0.0001
	Zinc	17	64.7	37	100.0	6	0.0001
SW061	Barium	50	82.0	42	95.2	2	0.0001
	Calcium	65	100.0	42	100.0	2	0.0001
	Lead	52	30.8	42	57.1	6	0.0499
	Lithium	49	57.1	42	54.8	6	0.0003
	Magnesium	60	90.0	42	100.0	2	0.0001
	Sodium	66	100.0	42	100.0	2	0.0001
	Strontium	54	85.2	42	95.2	2	0.0001
	Zinc	65	76.9	42	100	6	0.0001
SW132	Barium	50	82.0	32	100.0	2	0.0001
	Calcium	65	100.0	32	100.0	2	0.0001
	Lithium	49	57.1	32	65.6	6	0.0001
	Magnesium	60	90.0	32	100.0	2	0.0001
	Potassium	50	70.0	32	75.0	6	0.0001
	Selenium	46	8.7	32	62.5	6	0.0001
	Sodium	66	100.0	32	100.0	2	0.0001
	Strontium	54	85.2	32	100.0	2	0.0001

Table 3B OU2 TOTAL METALS - POTENTIAL CONTAMINANTS OF CONCERN

Site	Analyte	Standard ($\mu\text{g/l}$)	Background			Site		
			Sample Size	% Detects	Number of Exceedances	Sample Size	% Detects	Number of Exceedances
SW059	Cadmium	1.50	10	0.0	0	37	8.1	3
	Thallium	0.012	16	0.0	0	36	1.0	1
SW061	Cadmium	1.50	38	0.0	0	42	2.4	1
	Thallium	0.012	45	6.7	3	41	7.3	3
SW132	Cadmium	1.50	38	0.0	0	32	6.3	2
	Thallium	0.012	45	6.7	3	30	3.3	1

Table 3C
(First of three pages)

OU2 TOTAL METALS - OTHERS

Site	Analyte	Background		Site		COC Decision Class	p Value
		Sample Size	% Detects	Sample Size	% Detects		
SW059	Aluminum	15	80 0	37	81 1	4Le	0 3427
	Antimony	13	15 4	37	18 9	6	0 1643
	Arsenic	12	41 7	35	11 4	6	0 9795
	Beryllium	13	0 0	37	5 4	5	0 Exceed
	Cesium	14	7 1	35	11 4	6	0 7265
	Chromium	13	15 4	37	29 7	6	0 2316
	Cobalt	12	0 0	37	10 8	6	0 1758
	Copper	15	40 0	36	36 1	6	0 6474
	Iron	16	93 8	37	89 2	4Le	0 8365
	Lead	13	46 2	37	62 2	6	0 5102
	Lithium	14	71 4	37	78 4	6	0 6215
	Manganese	18	83 3	37	78 4	6	0 6104
	Mercury	13	15 4	37	16 2	6	0 5221
	Molybdenum	13	23 1	37	18 9	6	0 5371
	Nickel	12	8 3	36	30 6	6	0 1174
	Potassium	14	64 3	37	81 1	6	0 9548
	Selenium	14	21 4	37	18 9	6	0 6914
	Silicon	7	100 0	26	100 0	3	0 6860
	Silver	13	7 7	36	16 7	6	0 3349
	Tin	12	16 7	36	22 2	6	0 4050
	Vanadium	13	38 5	37	54 1	6	0 3436

Table 3C
(Second of three pages)

OU2 TOTAL METALS - OTHERS

Site	Analyte	Background		Site		COC Decision Class	p Value
		Sample Size	% Detects	Sample Size	% Detects		
SW061	Aluminum	56	69 6	42	66 7	6	0 8990
	Antimony	45	17 8	42	2 4	6	0 7231
	Arsenic	41	12 2	42	11 9	6	0 4928
	Beryllium	43	4 7	42	4 8	5	0 Exceed
	Cesium	45	4 4	42	7 1	5	0 Exceed
	Chromium	45	17 8	42	19 1	6	0 7689
	Cobalt	42	9 5	42	11 9	6	0 7937
	Copper	46	41 3	41	36 6	6	0 9209
	Iron	67	91 0	42	76 2	6	0 9706
	Manganese	61	88 5	42	95 2	2	0 0648
	Mercury	48	12 5	42	9 5	6	0 9000
	Molybdenum	49	14 3	42	16 7	6	0 9333
	Nickel	45	24 4	42	7 1	6	0 9795
	Potassium	50	70 0	42	76 2	6	0 1928
	Selenium	46	8 7	42	11 9	6	0 3074
	Silicon	20	100 0	34	100 0	2	0 3194
	Silver	43	7 0	42	14 3	6	0 2546
	Tin	42	19 1	42	7 1	6	0 9981
	Vanadium	44	27 3	42	38 1	6	0 1746

Table 3C
(Third of three pages)

OU2 TOTAL METALS - OTHERS

Site	Analyte	Background		Site		COC Decision Class	p Value
		Sample Size	% Detects	Sample Size	% Detects		
SW132	Aluminum	56	69.6	32	59.4	6	0.9990
	Antimony	45	17.8	32	3.1	6	0.5415
	Arsenic	41	12.2	32	18.8	6	0.5235
	Beryllium	43	4.7	32	6.3	5	0 Exceed
	Cesium	45	4.4	31	6.5	5	0 Exceed
	Chromium	45	17.8	32	9.4	6	0.9496
	Cobalt	42	9.5	32	6.3	5	0 Exceed
	Copper	46	41.3	31	22.6	6	0.9971
	Iron	67	91.0	32	87.5	2	0.9990
	Lead	52	30.8	31	61.3	6	0.0512
	Manganese	61	88.5	32	93.8	2	0.4103
	Mercury	48	12.5	32	25.0	6	0.1768
	Molybdenum	49	14.3	32	15.6	6	0.8284
	Nickel	45	24.4	31	3.2	6	0.9918
	Silicon	20	100.0	32	100.0	2	0.8557
	Silver	43	7.0	32	0.0	5	0 Exceed
	Tin	42	19.1	30	0.0	6	0.9991
	Vanadium	44	27.3	32	18.8	6	0.9464
	Zinc	65	76.9	32	81.3	6	0.1228

Table 4A

OU2 DISSOLVED METALS - CONTAMINANTS OF CONCERN

Site	Analyte	Background		Site		COC Decision Class	p Value
		Sample Size	% Detects	Sample Size	% Detects		
SW059	Barium	17	64.7	38	89.5	6	0.0001
	Calcium	17	100.0	38	100.0	3	0.0006
	Magnesium	17	94.1	38	100.0	4Ne	0.0001
	Sodium	17	100.0	38	100.0	3	0.0001
	Strontium	17	70.6	37	100.0	6	0.0001
	Zinc	14	50.0	38	100.0	6	0.0001
SW061	Barium	63	55.6	42	95.2	6	0.0001
	Calcium	66	100.0	42	100.0	2	0.0001
	Lithium	52	44.2	41	56.1	6	0.0004
	Magnesium	64	79.7	42	100.0	6	0.0001
	Manganese	62	61.3	42	92.9	6	0.0001
	Potassium	53	60.4	41	75.6	6	0.0445
	Sodium	66	98.5	42	100.0	2	0.0001
	Strontium	60	70.0	41	95.1	6	0.0001
SW132	Arsenic	35	0.0	28	39.3	6	0.0009
	Barium	63	55.6	32	96.9	6	0.0001
	Calcium	66	100.0	32	100.0	2	0.0001
	Lithium	52	44.2	32	59.4	6	0.0001
	Magnesium	64	79.7	32	100.0	6	0.0001
	Manganese	62	61.3	32	84.4	6	0.0005
	Potassium	53	60.4	32	75.0	6	0.0001
	Selenium	34	0.0	32	62.5	6	0.0001
	Sodium	66	98.5	32	100.0	2	0.0001
	Strontium	60	70.0	32	100.0	6	0.0001

Table 4B
(First of three pages)

OU2 DISSOLVED METALS - OTHERS

Site	Analyte	Background		Site		COC Decision Class	p Value
		Sample Size	% Detects	Sample Size	% Detects		
SW059	Aluminum	14	28 6	38	36 8	6	0 1881
	Antimony	10	40 0	38	21 1	6	0 8930
	Arsenic	12	33 3	37	10 8	6	0 9821
	Beryllium	4	0 0	38	2 6	5	0 Exceed
	Cadmium	6	0 0	38	2 6	5	0 Exceed
	Cesium	8	0 0	36	5 6	5	0 Exceed
	Chromium	7	14 3	38	23 7	6	0 4084
	Cobalt	7	0 0	38	7 9	5	0 Exceed
	Copper	15	46 7	37	21 6	6	0 9888
	Iron	17	47 1	37	32 4	6	0 9665
	Lead	14	14 3	38	21 1	6	0 1040
	Lithium	17	58 8	37	64 9	6	0 8481
	Manganese	17	70 6	38	55 3	6	0 9309
	Mercury	5	40 0	38	5 3	6	0 9619
	Molybdenum	10	30 0	37	24 3	6	0 9028
	Nickel	7	14 3	38	10 5	6	0 8802
	Potassium	14	50 0	38	76 3	6	0 7469
	Selenium	8	12 5	37	16 2	6	0 7429
	Silicon	7	100 0	27	100 0	3	0 9495
	Silver	8	12 5	36	13 9	6	0 5437
	Thallium	8	0 0	36	0 0	5	0 Exceed
	Tin	10	20 0	36	22 2	6	0 8157
	Vanadium	12	25 0	38	31 6	6	0 4257

Table 4B
(Second of three pages)

OU2 DISSOLVED METALS - OTHERS

Site	Analyte	Background		Site		COC Decision Class	p Value
		Sample Size	% Detects	Sample Size	% Detects		
SW061	Aluminum	54	42.6	42	31.0	6	0.9868
	Antimony	42	21.4	42	2.4	6	0.8883
	Arsenic	35	0.0	41	9.8	5	0 Exceed
	Beryllium	36	8.3	24	5	5	0 Exceed
	Cadmium	30	0.0	42	4.8	5	0 Exceed
	Cesium	38	5.3	41	4.9	5	0 Exceed
	Chromium	34	5.9	42	11.9	6	0.5096
	Cobalt	35	0.0	42	4.8	5	0 Exceed
	Copper	58	34.5	41	22.0	6	0.9998
	Iron	65	66.2	41	41.5	6	0.9999
	Lead	47	23.4	41	31.7	6	0.2865
	Mercury	31	9.7	42	2.4	5	0 Exceed
	Molybdenum	40	12.5	40	17.5	6	0.9897
	Nickel	40	2.5	42	9.5	5	0 Exceed
	Selenium	34	0.0	42	21.4	6	0.0607
	Silicon	20	100.0	35	100.0	2	0.7151
	Silver	37	5.4	41	7.3	5	0 Exceed
	Thallium	41	4.9	40	2.5	5	0 Exceed
	Tin	43	14.0	41	2.4	6	0.9987
	Vanadium	44	15.9	42	28.6	6	0.0588
	Zinc	62	61.3	42	47.6	6	0.7993

Table 4B
(Third of three pages)

OU2 DISSOLVED METALS - OTHERS

Site	Analyte	Background		Site		COC Decision Class	p Value
		Sample Size	% Detects	Sample Size	% Detects		
SW132	Aluminum	54	42.6	31	22.6	6	0.9943
	Antimony	42	21.4	32	9.4	6	0.8269
	Beryllium	36	8.3	32	6.3	5	0. Exceed
	Cadmium	30	0.0	32	3.1	5	0. E exceed
	Cesium	38	5.3	32	18.8	6	0.6866
	Chromium	34	5.9	32	6.3	5	0. Exceed
	Cobalt	35	0.0	32	3.1	5	0. E exceed
	Copper	58	34.5	31	25.8	6	0.9987
	I on	65	66.2	32	31.3	6	0.9999
	Lead	47	23.4	29	31.0	6	0.2891
	Mercury	31	9.7	32	9.4	5	0. Exceed
	Molybdenum	40	12.5	32	18.8	6	0.9902
	Nickel	40	2.5	32	6.3	5	0. Exceed
	Silicon	20	100.0	32	100.0	2	0.8776
	Sil er	37	5.4	32	0.0	5	0. E exceed
	Thallium	41	4.9	30	3.3	5	0. Exceed
	Tin	43	14.0	31	0.0	6	0.9999
	Vanadium	44	15.9	32	3.1	6	0.9860
	Zinc	62	61.3	31	32.3	6	0.9990

Table 5

OU2 WATER QUALITY PARAMETERS

Site	Analyte	Background		Site		COC Decision Class	p Value
		Sample Size	% Detects	Sample Size	% Detects		
SW059	Chloride	18	88.9	37	100.0	3	0.0001
	Total Organic Carbon	3	100.0	23	100.0	4Le	0.9988
SW061	Chloride	68	88.2	39	100.0	2	0.0001
	Total Organic Carbon	11	100.0	29	100.0	3	0.9974
SW132	Chloride	68	88.2	28	100.0	2	0.0001
	Total Organic Carbon	11	100.0	27	96.3	3	0.9808

For each site these p Values indicate that Chloride is a COC. Total Organic Carbon is not a COC for any of the sites and is in fact at significantly lower levels in each site than in the background.

Explanation of Scores Methodology

In a standard Mann-Whitney/Wilcoxon application two samples which are to be compared are combined into a single sample and the observations are then ranked as a single sample. The ranks resulting from one of the two samples are then summed to see if they generally were larger or smaller than would be expected if the samples were taken from the same distribution. If so the null hypothesis of no differences in the two underlying distributions would be rejected in favor of an alternative hypothesis of one distribution being shifted with respect to the other.

As a simple example consider the following where a one-sided test of whether the sample 2 values come from a distribution of larger values is of interest.

Sample 1 1 4 5 7 12 15

Sample 2 4 8 17 18

The combined sample is then 1 4 4 5 7 8 12 15 17 18

with respective ranks 1 2 5 2 5 4 5 6 7 8 9 10

The sum of the ranks for the second sample is therefore $2 + 5 + 6 + 9 + 10 = 27.5$ (note that tied values receive average ranks). This rank sum of 27.5 is compared to values expected under the null hypothesis of equal distributions to determine if the sum is sufficiently large to be deemed statistically significant.

The Mann-Whitney/Wilcoxon approach can be applied to censored data only if the censoring values are smaller than all detects. In this case all nondetects would be treated as tied.

The situation gets more complicated when multiple detection limits (censoring values) are present in the two samples. Not all values can then be ranked with respect to each other. For example, it is unknown whether a nondetect with a detection limit of 10.0 is greater or less than a detect at 5.0, so their relative ranks cannot be determined. Similarly, the ranking of two nondetects with different detection limits cannot be determined.

One simple approach for determining a ranking of such data that has been suggested in statistical literature is to treat every measurement that is less than the largest nondetect as a tied value whether it is a detect or a nondetect. This clearly has the shortcoming of not using all the information that is available. For example, with nondetects at 5.0 and 10.0 and a detect at 7.5, it is known that the 7.5 valued detect is clearly greater than the nondetect at 5.0. This information would be ignored in this approach.

An improvement is given in Millard and Deveral (1988). The scores approach proposed in this report is developed in that paper. While several variations are discussed, they generally behave comparably. The Gehan variation is proposed for use in this report largely since its derivation is the simplest to understand.

To see how the scores approach works consider another example The notation <12 represents a nondetect at the detection limit of 12 and therefore a value less than 12 0

Sample 1 1 <4 5 7 <12 15

Sample 2 2 <4 8 17

This gives the combined sample as 1 2 <4 <4 5 7 8 <12 15 17

Although the scores approach is not specifically defined in terms of ranking it can most easily be explained in terms of the ranks it equivalently ends up generating Again it is analogous to the Mann-Whitney/Wilcoxon approach and equivalent to it in the presence of no nondetects The rankings for the scores method occur as follows They are most easily assigned from largest to smallest

The values 17 and 15 get ranks 10 and 9 respectively as they are known to be the two largest values even with the presence of nondetects

The <12 value is taken to be tied with all seven values below it and thus receives as its rank the average of the ranks 1 to 8 which is 4.5

The value 8 is clearly greater than the six values below it and clearly less than the values 15 and 17 It is treated as a tie with the value <12 and therefore receives the average of the ranks 7 and 8 which is 7.5

The value 7 is clearly greater than the five values below it and clearly less than the values 8, 15, and 17 It is treated as a tie with the value <12 and therefore receives the average of the ranks 6 and 7 which is 6.5

The value 5 is clearly greater than the four values below it and clearly less than the values 7, 8, 15, and 17 It is treated as a tie with the value <12 and therefore receives the average of the ranks 5 and 6 which is 5.5

The two values <4 are clearly less than the values 5, 7, 8, 15, and 17 and are treated as tied with each other as well as with the values 1, 2, and <12 They therefore receive the average of the ranks 1, 2, 3, 4, and 5 which is 3

The value 2 is clearly greater than the value 1 and clearly less than the values 5, 7, 8, 15, and 17 It is treated as a tie with the values <4, <4, and <12 and therefore receives the average of the ranks 2, 3, 4, and 5 which is 3.5

The value 1 is treated as tied with the values <4, <4, and <12 and therefore receives the average of the ranks 1, 2, 3, and 4 which is 2.5

In summary the following ranking results

Sample values	1	2	<4	<4	5	7,	8	<12	15	17
Ranks	2.5	3.5	3	3	5.5	6.5	7.5	4.5	9	10

Note that with no ties or nondetects in this example the sum of the resulting ranks 1 2 10 would be 55. The sum of the scores ranks in the example is also 55. This is always a property of this scores ranking scheme.

The test statistic as in the Mann-Whitney/Wilcoxon approach can be considered as the sum of the ranks of the sample values from one of the samples. If the sample used is the site sample then large values of this statistic would indicate that the site is generating samples that are large relative to the background samples and the associated analyte would be classified as a COC.

Distributional properties for the statistic can be obtained through the usual approach used for rank methods. This considers all permutations of the resulting rankings since all such permutations are equally likely under the null hypothesis of no difference in the underlying site and background populations. If the statistic takes on a value in the upper five percent of the resulting values it would be taken as statistical evidence that the analyte is elevated in the site relative to background and is therefore considered a COC. Note that this would provide the standard 0.05 Type I error probability (see the Type I error discussion on page 27).

The statistic used in the scores approach belongs to a nonparametric family called linear rank statistics (see Gibbons (1971)). Large sample normal approximations to the distributions of such statistics have been shown to be appropriate even for fairly moderate sample sizes. This approximation is therefore appropriate in the applications of this report and has been used.

Changes in Results for Scores Only Approach

Various statistical hypothesis tests have been used in this report to identify COCs. All of COC Decision Classes 2, 3, 4, and 6 are in this category. The nonparametric censored data scores test is an appropriate statistical tool for every one of these cases. In fact, with no nondetects as mentioned earlier, this test is equivalent to the Mann-Whitney/Wilcoxon test. The scores test was applied to all cases for COC Decision Classes 2, 3, and 4 to determine if any differences in COC determinations would have occurred.

The only difference obtained was for Manganese in Total Metals. This was not found to be a COC under the central limit theorem approach of COC Decision Class 2. However, two outlying values in the background data and one in the site data had considerable influence on the t-test used. In fact, if the data had first been log transformed or if the outlying values had been omitted, this analyte would have been determined to be a COC under the central limit theorem approach as well. Since the nonparametric scores approach is less sensitive to outlying values, it makes the COC determination using the original data. In no other case for RADS total metals, and dissolved metals was a different COC or non-COC determination obtained by using the nonparametric scores approach.

This comparison illustrates that the scores approach is an adequate method for application in general. It is robust for any underlying distribution, large numbers of nondetects, multiple detection limits, and outlying values. It reduces to the Mann-Whitney/Wilcoxon approach in the presence of no nondetects. In addition, the extensive, fairly tedious, and less statistically rigorous series of analysis steps involved in applying the flow chart could be avoided.

Type I and Type II Errors

In statistical hypothesis testing a null hypothesis which includes equality is specified and tested against an appropriate alternative hypothesis. Type I errors and Type II errors are associated with such testing. A Type I error consists of rejecting the null hypothesis in favor of the alternative hypothesis when in fact the null hypothesis is true. A Type II error consists of accepting the null hypothesis rather than the alternative hypothesis when in fact the null hypothesis is false. The probability of a Type I error is controlled during the testing at a low level (commonly 0.05). The probability of a Type II error is then uncontrolled but for a specified Type I error probability the Type II error probability decreases with increasing sample sizes and will go to zero for very large sample sizes. Note that the power of the test is the ability to correctly reject the null hypothesis in favor of the alternative hypothesis when the null hypothesis is false. The power is therefore one minus the probability of committing a Type II error.

For a background to site comparison for the determination of a COC a Type I error consists of incorrectly determining an analyte to be a COC when in fact it should not have been. A Type II error is failing to identify an analyte as a COC when in fact it should have been so identified. The power is therefore the probability of correctly identifying a COC. The relative costs and risks associated with making Type I and II errors should be considered especially when selecting an appropriate Type I error probability level.

For all statistical comparisons in this report a p-value is generated. P-values are between 0.0 and 1.0 with small values indicating differences and that the alternative hypothesis should be favored over the null hypothesis. If a p-value is less than 0.05 for this report the associated analyte is taken to be a COC. Note as well that large p-values would in fact indicate that the background contains higher levels of an analyte than the site.

Note that the practice of treating several site locations individually as single sites rather than grouping them into one overall site for comparison to background will increase the overall likelihood of making Type I errors while decreasing the probability of making Type II errors. A 0.05 Type I error probability will exist for each location rather than a single overall 0.05 Type I error for the combined locations. However differences between site locations and the difficulty in doing multiple location comparisons in the presence of many nondetects with multiple detection limits generally necessitate the individual locations approach.

Use of Tolerance Limits

Inference based on tolerance intervals involves estimation of tail behavior of distributions. Such estimation is much more dependent on underlying distributions, sample sizes, nondetects, multiple detection limits, and outliers than the considerably simpler task of estimating means, medians, or standard deviations. Tolerance interval limit estimators, especially for this type of environmental data, are extremely volatile and sensitive to the data problems.

Equally important is the issue of how the tolerance intervals would be used for comparisons to background even with well-behaved normally distributed data (or

for that matter nonparametric tolerance intervals for non-normal data) Loftis, et al (1986) suggests using background data from wells to establish tolerance limits, but then recommends that future observations considered one at a time from a site well be compared to the tolerance limits (see example page 91 of that paper) Over time as long as the site well measurements are within limits, the site well is in compliance When a measurement is found to be outside the limits, the site well at that time is taken to be out of compliance This is a reasonable application of tolerance limits but it is simply a control charting type application to evaluate an ongoing sequence of measurements

U S EPA (1989) discusses a similar approach but points out that any one of tolerance limits prediction limits, and control chart limits could be used for such a control charting application The text on page 5-22 includes the statement Compare each observation from compliance wells to the tolerance limit

This discussion is somewhat vague but SA personnel believe the intent is the future observations one at a time type of application discussed above This is the approach in the example on page 5-23, wells are out of compliance in the months when values are obtained outside of the tolerance limits

An example on page 55 in U S EPA (1992) is even more vague and uses the words Compare each sample from the compliance wells to nonparametric tolerance limits However the data in this example is also ordered by month so the intent is still thought to be the one-at-a-time application

Thus at no time is a tolerance interval approach proposed by the EPA that generates tolerance limits from background data and then compares a group (unordered) of measurements from a site Such an approach is essentially unworkable Something like five percent of data is expected to fall outside of a 95/95 one-sided tolerance interval even for the background data on which it was based Say that the convention is accepted that any one measurement from the site falling above the upper tolerance is sufficient to declare the analyte as a COC in the site Even if the site is not different from background something like five percent of data should fall above the limit Maybe none will for quite small sample sizes, but as sample sizes increase only moderately it is guaranteed that some will fall outside the interval five percent should! Thus even backgrounds, when retested would generate COC conclusions Type I error probabilities are much larger than 0.05 even for small sample sizes and go to 1.0 as sample sizes increase

Say instead that the COC determination will be made only if more than five percent of the site data fall outside the limit (this is a somewhat more reasonable intuitive approach) Then however since five percent are expected to fall above the limit the chance of getting more or less than the five percent is a 50/50 proposition The Type I error probability is now theoretically about 0.5 obviously unacceptably high

To use tolerance limits the Type I error would have to be reduced One could require maybe 10 percent of site data to exceed a 95/95 tolerance limit to make a COC determination Obviously this doesn't sound very appealing and it's still not clear how one would then quantify the Type I error

In conclusion comparing a site data set to tolerance limits computed from background is simply not a very reasonable approach it cannot be defended from

a statistical standpoint. It is reasonable for a control charting application with data being obtained over time, but even in that case use of tolerance limits is possibly overly rigorous when compared to the typical control charting applications of statistical process control methodology commonly used in manufacturing. Such control charting methods are not the methods needed for COC determination through the comparison of two data sets.

Conclusions

A branching flow chart for determining appropriate statistical methodology for comparing site and background data for the determination of COC's is provided. The methodology is applied to seep and stream locations in OU2 tables of COC and non-COC results are given. It is recommended that a nonparametric scores approach, which is used for the multiple detection limit case in the flow chart, be used in all cases instead of the other statistical approaches discussed.

The tolerance interval approach should not be used for comparing site and background data sets since the corresponding Type I error probabilities can be neither computed nor controlled. Therefore the results are not particularly meaningful in this context, are not statistically defensible, and would be especially vulnerable to successful challenge at the time of public comment.

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